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Meeting Reports

The canSAS-IV Meeting at Diamond / ISIS

The Fourth in the occasional series of *canSAS* meetings took place at the Rutherford Appleton Laboratory (RAL), UK, over May 12-14, 2004.

canSAS - Collective Action for Nomadic Small-Angle Scatterers - was conceived at the ILL/ESRF campus in 1998 as a means to try to alleviate some of the problems that beset visiting users of small-angle scattering (SAS) instruments at neutron and X-ray facilities due to differences in the data formats. It seemed that every facility, and in some cases almost every instrument, had its own format for essentially the same information! In addition this had given rise to a plethora of data analysis programs, often performing the same calculations. The inaugural canSAS meeting wanted to see if there might be ways to reduce the entropy of the situation, provide a "point of contact" where information might be deposited and shared, and foster interaction between the neutron and X-ray halves of the SAS Community around the world; see *Neutron News*, **9(3)**, 6, (1998).

In this role canSAS has actually been reasonably successful (if a little anonymous), although progress on the thorny issue of data formats has perhaps not been as swift as many would like.

One of the other factors affecting the SAS Community in recent years has been the rapid growth in what might be termed "added-value" experiments; for example, the coupling of DSC with SAXS/WAXS, rheometric measurements with SANS, and the in-situ use of stop-flow apparatus, stress rigs and extruders, to name but a few. Such experiments not only generate large multi-parameter datasets, but are increasingly also being done in real-time (even with today's relatively low flux neutron sources). All this naturally has serious implications for data acquisition and data handling, particularly on tomorrow's sources.

It was against this backdrop that 60 delegates, 33 of whom were from overseas (including Australia, Japan and the US), gathered for what turned out to be a very successful and lively meeting. Indeed, the organisers had to close registration early because the room capacity had been reached!

Crammed into a very busy two-day programme were 25 oral presentations, almost as many poster presentations, half a dozen software demonstrations, a tour of ISIS, and the opportunity to see the new Diamond Light Source under construction!

canSAS-IV formally commenced with an address by Andrew Taylor, Deputy Chief Executive of CCLRC and Director of ISIS, who spoke about the future opportunities for soft matter research that would present themselves on completion of the Diamond Synchrotron (2006) and the ISIS Second Target Station (2007). There were also expected to be significant enhancements of the campus infrastructure to go alongside these major investments in scientific facilities.

Meeting contributions then largely addressed three areas: new technical developments, software developments, and "cutting-edge" science embracing one or other (or perhaps both!) of the above.

Elliot Gilbert (Bragg Institute, ANSTO) gave a review of the recent meeting at Lucas Heights on "Data Visualisation, Reduction and Analysis at Australia's Replacement Research Reactor". This had emphasised the key role that well-written, intuitive, tested, software plays in turning experimental data into meaningful scientific results, and encouraged the establishment of a central repository of routines conforming to an established framework.

Jun-ichi Suzuki (JAERI, Tokai) then explained how polarised neutron beams could be focussed by magnetic "lenses". The significance of this approach for SANS is that there is only a 50% flux loss (assuming 100% polarisation) regardless of the Q-vector being targeted, whereas in a conventional (pinhole) SANS instrument the loss of flux at small Q is quite severe because of the need for highly-collimated beams and long sample-detector distances. The magnetic lens approach is also applicable to time-of-flight (TOF) SANS. A drawback, of course, is the cost of the magnets!

Michael Drakopoulos (Diamond, Didcot) followed a similar theme and discussed the use of compound refractive lenses with X-rays. This talk illustrated how such optical

elements have opened up fields such as SAXS Microscopy and X-ray Imaging.

Wim Bras (DUBBLE, Grenoble) highlighted how software performing even relatively unsophisticated data treatments has largely failed to keep pace with the growth in data volume due to time-resolved SAXS. Quite simply, only a few percent of the time-resolved data collected at synchrotrons around the world is ever "analysed". Whilst considerable resources are directed into beam line and detector developments, far fewer resources seem to be directed at making more efficient use of the data that can be collected right now. Though the problem is more acute in SAXS, it also affects SANS.

Thomas Weiss (ESRF, Grenoble) demonstrated how putting a Daresbury SRS RAPID detector on the high-brilliance ID2 beam line at the ESRF, together with stop-flow apparatus, had enabled them to elucidate the kinetics of the micelle-to-vesicle transition in an anionic/zwitterionic surfactant mixture. Data was recorded with millisecond time resolution.

Charles Dewhurst (ILL, Grenoble) gave an overview of his MatLab script GUI GRAS$_{ans}$P for SANS multidector data, illustrating its graphical capabilities on some early data from the recently installed D22 linear multidetector array of 8 mm diameter, 1 m long gas tubes. Count rates of up to 3 MHz have already been realised. It is necessary to both geometrically calibrate and correct for non-linearity at the ends of the tubes in software. This has led to much discussion about what constitutes the "raw" data, and how it should be stored.

Stepping in to fill a vacant slot at very short notice, *Rob Dalgliesh (ISIS, Didcot)* talked about the opportunities presented by the emerging field of Spin-Echo SANS (SESANS). In a presentation that Rob duly acknowledged as primarily the work of others, he explained how SESANS was an alternative means for accessing larger length scales (*cf.* the double-crystal/Bonse-Hart or magnetic lens approaches) but in *real space*, not Q space. A purpose-built instrument already exists at IRI in The Netherlands and ISIS is looking into the feasibility of adapting the technique to a pulsed source.

Theyencheri Narayanan (ESRF, Grenoble) gave an elegant overview of Ultra-SAXS (USAXS), including how the partially coherent nature of synchrotron X-radiation may be exploited in the emerging technique of Dynamic-USAXS (*cf.* Photon Correlation Spectroscopy) for the study of colloidal systems.

Jan Šaroun (Nuclear Physics Institute, Prague) then presented details of his SASProFit software for the combined modelling of USANS and SANS data, illustrating its capabilities with a case study of cavity formation in a superplastic alloy.

Though not a "scatterer" in any sense of the word, *Elena Pourmal (NCSA, Urbana-Champaign)* has been a welcome visitor to more than one canSAS meeting in her capacity as a lead developer of HDF5, the Hierarchical Data Format, the "tool" that underlies the NeXus file format. In her talk Elena charted the challenges in data management that gave rise to HDF, an overview of its current usage (the NASA Earth Observation System archive alone currently stands at 4M Gb, dwarfing anything the neutron and X-ray communities are likely to achieve!), and looked to the future (e.g. client-server adaptations for GRID applications, the rise of bioinformatics and, worryingly, an uncertain funding model).

Ron Ghosh (ILL, Grenoble) is one of the canSAS "founding fathers". He was also the ideal person to take the audience back through time to show how some of the present problems in respect of data formats and the difficulties of sharing and visualising data across facilities have evolved. There were a number of insightful observations: the platform dependence of many current GUI's, libraries and executables; that, whilst platform independent, Python and Java have rather poor math libraries; that many of the commercial packages have different scripting languages; and that, increasingly, *Users do not, can not, or will not, program*. Ron also presented his vision for the future, a "data query language" for data files (*cf.* SQL for databases).

Rainer Wilcke (ESRF, Grenoble) returned to the problems facing time-resolved SAXS, reminding the audience, in particular, that the true data quality (statistics) could only be properly estimated after initial corrections. At the ESRF a program has been developed to automatically apply these corrections online within seconds of data acquisition, even for time-resolved data.

Rex Hjelm (LANSCE, Los Alamos) talked about some of the pitfalls and benefits they had experienced with new data acquisition, instrument control and data management systems on the LQD SANS instrument following its recent upgrade. This instrument is one of the very few to have actually implemented a NeXus raw file format (albeit a non-standard implementation) and it was encouraging to hear that it seems to have found favour.

Bill Pulford (Diamond, Didcot), the newly installed Head of the Data Acquisition (DAQ) Group, outlined the basic ideas that he was promoting for Diamond. Whilst control of the accelerator and the beam lines will be provided by EPICS (as at the APS), DAQ and experiment control will use Java with Jython as a scripting language. It is expected that raw data will be stored in the NeXus format, and there was a strong commitment towards the use of electronic logs and "beam line configuration databases". Bill also envisaged Terabyte disk arrays in each experimental station and having a scientific programmer "associated" with each scientific technique. The X-ray community sees this level of resource allocation as essential in the

future.

Kevin Knowles (ISIS, Didcot), Head of the ISIS Computing Group, gave the view "from the other side of the road" (literally!). ISIS has been steadily migrating from VMS/Q-Bus based DAQ systems, to OpenVMS/SCSI based systems, and latterly to PC/VME based systems, with scripting through the ISIS OpenGenie package. LabView® is gradually replacing CAMAC for control of beam line instrumentation and sample environment.

Dmitri Svergun (EMBL, Hamburg) presented details of the latest enhancements to the ATSAS program suite for the analysis and modelling of solution SAS data: a program (PRIMUS) for initial data treatment, and for the biological community a database (DARA) of SAS curves computed from the PDB.

Tracy Nixon (Pennsylvania State University) introduced himself as a cell biologist who is interested in how AAA+ ATPases couple ATP hydrolysis with mechanical work and, thus, conformational change. A speculative enquiry led to some casual beam time at the APS BioCAT beam line and an introduction to Dmitri Svergun's programs, and now he is a convert to SAXS/WAXS! This was an excellent and refreshing tale from someone who was now sold on the benefits of SAS.

Adrian Rennie (NFL, Studsvik) is another *canSAS* stalwart and, as both an ex-instrument scientist and ex-academic, is someone well-qualified to judge how both sides view SANS experiments. What makes an experiment difficult from the instrument responsible's perspective (often something about the sample) is usually completely different to the Users perspective (the problem is with the instrument)! To illustrate this Adrian showed two examples from his own work on optoelectronic materials: a cadmium chalconide borosilicate glass, and a spin-coated film of organic photoluminescent polymer 100 nm thick (corresponding to an illuminated sample mass of just 0.02 mg) - neither are instinctive samples for a SANS experiment.

Aymeric Robert (ESRF, Grenoble) talked about the TROIKA beam line at the ESRF and X-ray Photon Correlation Spectroscopy (XPCS). XPCS probes the same time domain as optical PCS but does so at higher Q values. Multiple scattering is also much less of a problem in XPCS and can, of course, be used to study "cloudy" or opaque samples. Unfortunately experience suggests that there is insufficient electron density contrast in typical protein solutions to make the technique attractive to the Life Sciences, whilst radiation damage to the sample is also something of a problem.

Xiangbing Zeng (University of Sheffield) described a real-time SANS study of isothermal crystallisation in a selectively-deuterated model alkane system, performed on LOQ at ISIS. Using a Temperature-Jump apparatus (~1 s jump) that also triggered the data acquisition, good quality data was recorded in frames as short as 10 s on as little as 100 mg of sample. An exciting development for SANS.

John Ramsay (CNRS, University of Montpellier II) described work on organically-directed colloidal zeolite particles for use in separation membranes and sensors. The particles form under hydrothermal conditions and the structure evolution was followed *in-situ* by WAXS, SAXS and USAXS on ID2 at the ESRF. Parallel SANS studies on another zeolite system exploited selective deuteration and contrast variation to gain an insight into the role of the organic cation, nicely complementing the X-ray work.

Kerstin Kleese-van-Dam (CCLRC e-Science Centre, Daresbury) gave an overview of what e-Science was ("a holistic approach to integration from the experiment to the results"), how it was likely to affect large-facilities and their Users in the future (remote-control or remote-supervision of experiments, better number-crunching, and better data archiving to name but a few), and a walk through some of the current projects: (The) GRID (essentially the utilisation of spare computing resources around the world), AccessGRID (like video-conferencing but over the web), DataPortal (a "one-stop shop" to access data across many locations), Storage Resource Broker (a truly global distributed file system), and the Digital Curation Centre. However, the question of who "owns" the data that is collected appears to be a matter of some debate.

William Helsby (CCLRC, Daresbury) from the CCLRC Instrumentation Department talked about the development, construction and operating principles of multi-wire gas detectors for both neutron and X-ray use. Highly-parallel readout systems provide much-demanded improvements in count rate performance. The new Daresbury High-Overall Throughput WAXS (HOTWAXS) detector, for example, has a global count rate of 500 MHz. Looking to the future there are several potential benefits (e.g. cost, counting accuracy & spatial resolution) from the developing field of micro-pattern detectors.

Richard Heenan (ISIS, Didcot) described work he had been involved with on D22 using the ILL Stop-Flow apparatus to follow a vesicle-to-micelle transition in a mixed surfactant system at, typically, just 5 mM concentration. In contrast to Thomas Weiss' millisecond time resolution achieved with X-rays (see above), the SANS data was recorded in 2 second frames, repeated 4 or more times to aggregate the statistics. This was a firm reminder, if one were needed, of just how great the difference in count rates between synchrotron SAXS and SANS still are. But from the SANS perspective, given the low scattering cross-sections, this work represents a great step forward in what can be achieved.

Rounding off the oral presentations, *John Squire (Imperial College, London)*, the current Chairman of CCP13, talked about the history of the project, its current status, and its possible future directions. Established to provide software for the analysis of (largely X-ray) fibre diffraction data, CCP13 has gradually broadened its remit to embrace polymers, oriented colloidal systems and the neutron community. Discussions are now underway to provide good model-fitting software for solution scattering.

There were two Discussion Sessions at *canSAS-IV*; one specifically on data file formats, the other on matters of more general interest to the SAS Community.

Freddie Akeroyd (ISIS) and Ken Littrell (IPNS) initiated the data file format discussion with two short presentations. Freddie - a member of the NeXus International Advisory Committee (NIAC) - gave an overview of the current status of NeXus. After a long (some might say overly long) gestation the formation of the NIAC in early 2003 seems to have given the project much-needed impetus. Agreement on NeXus "class" names, and on many of the item names within, should be completed by the end of June 2004 at which point the Instrument Definition "editors" (e.g. monochromatic neutron/X ray SAS and TOF neutron SAS) can start work. There was consensus amongst the audience for facilities to convert to NeXus as a raw data format.

Ken focussed more on issues to do with treated data, highlighting how almost every SAS instrument has an ASCII output format for its 1-dimensional (i.e. regrouped, azimuthally-averaged) data that consists of a header followed by some columns of numbers; yet every single one is different! It was proposed that *canSAS* should solicit a convergence to a common format. A further issue that was identified was the general absence of Q-error bounds in these treated data files.

The general discussion session focussed on building Community participation in *canSAS* and on the posture between canSAS and the IUCr Commission on Small-Angle Scattering (CSAS). Some in the audience thought that *canSAS* was doing what CSAS ought to be doing or, at least, doing more visibly.

Finally, it was proposed that it would be appropriate for *canSAS-V* to take place alongside the IUCr-sponsored SAS conference in Japan in 2006.

The organisers would like to express their gratitude to Diamond and ISIS (CCLRC), the ILL, and the DUBBLE (NOW/FWO) beam line at the ESRF for financial support.

The *canSAS* website is hosted by the ILL at the URL: http://www.ill.fr/lss/canSAS/. Additional contributions from the Community are encouraged. The abstracts for canSAS-IV are available online, as are a number of presentations and software downloads.

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